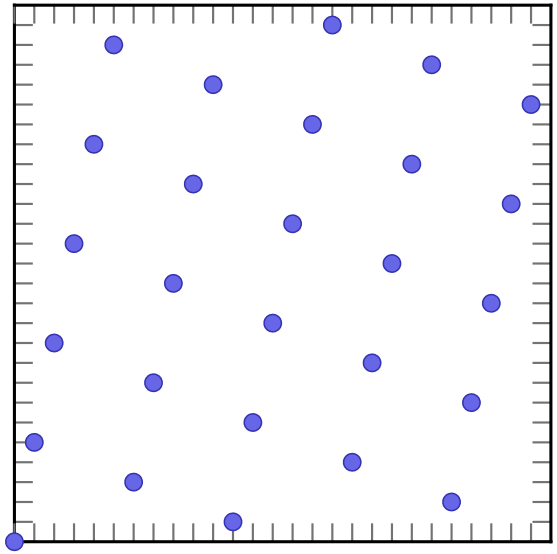
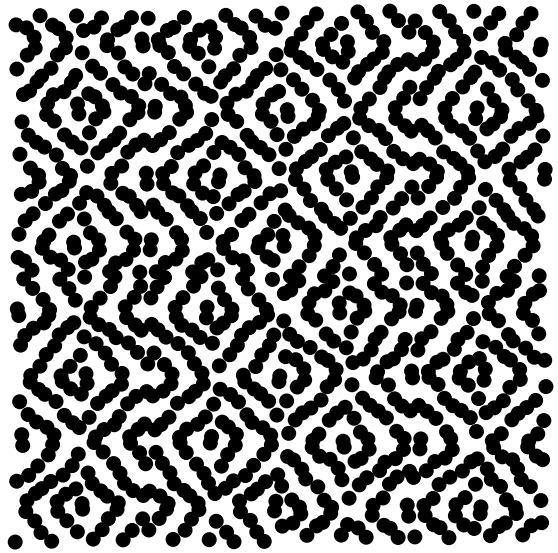
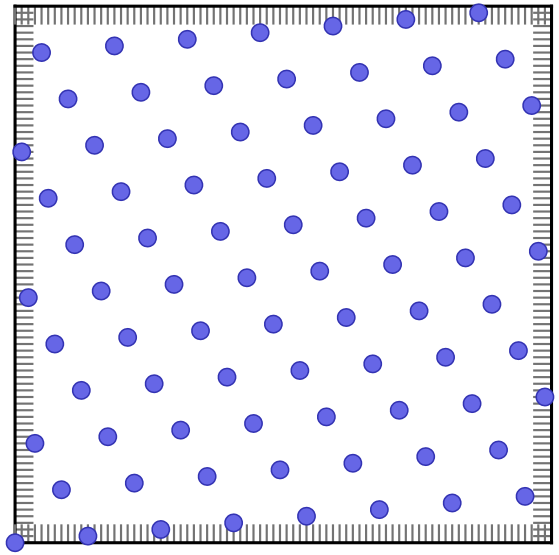
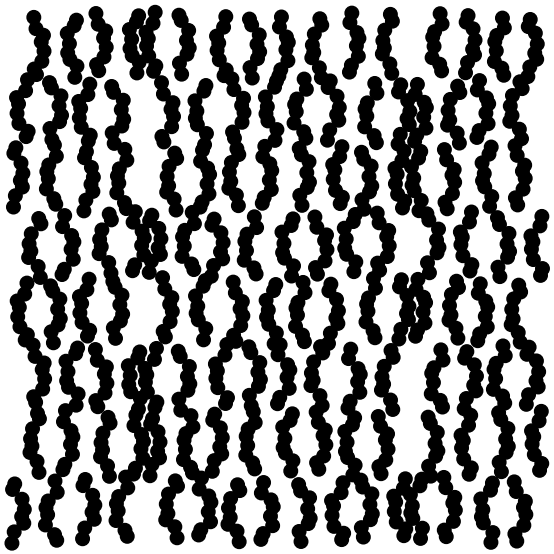
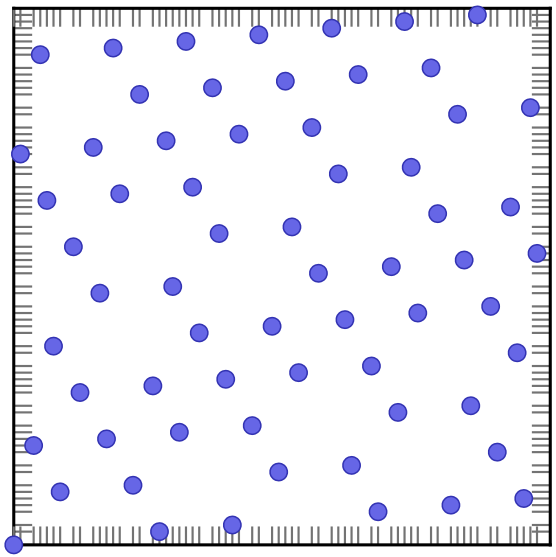
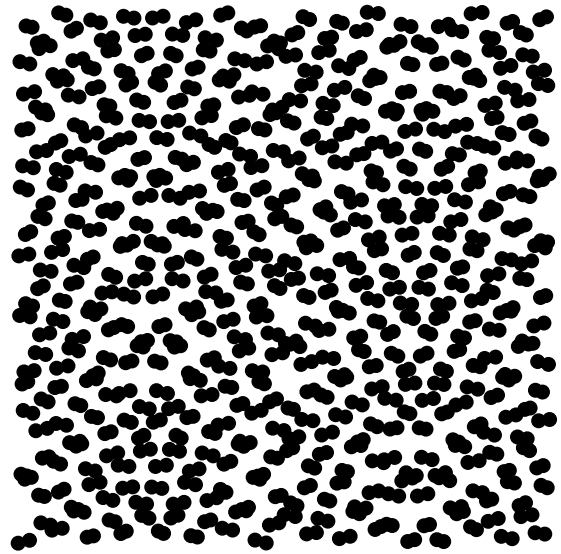




Lattice rules and beyond. . .

— Dirk Nuyens —

*Numerical Analysis and Applied Mathematics, Department of Computer Science, KU Leuven, Belgium • MCQMC2016, Stanford, August 14–19, 2016

High-dimensional integrals

Task: Approximate a d-dimensional integral

$$\mathbb{E}[f] = I(f) := \int_{\mathbb{R}^d} f(\boldsymbol{x})\, p(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} = \int_{[0,1]^d} f(P^{-1}(\boldsymbol{x}))\, \mathrm{d}\boldsymbol{x}.$$

Method: An N-point cubature/quadrature method

$$Q(f) = Q_N(f) = Q(f; \{(w_k, \boldsymbol{x}_k)\}_{k=1}^N) := \sum_{k=1}^N w_k\, f(\boldsymbol{x}_k).$$

(This talk: Using functional analysis and number theoretic uniform point sets. To tackle integration, approximation and "other" high dimensional problems.)

Applications: random fields, parametrised PDEs, financial engineering, Bayesian integrals, uncertainty quantification,...

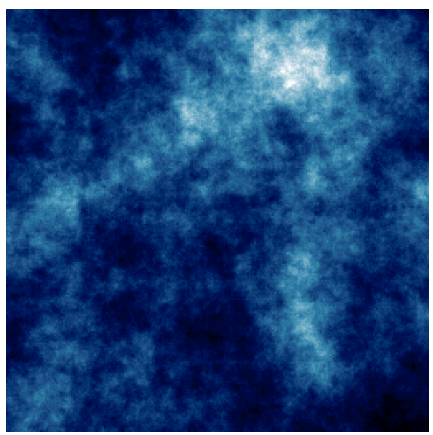
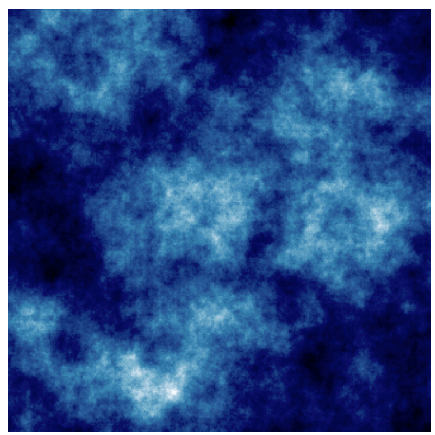
Example: random fields / parametrised PDEs ($d = \infty$)

Parametric representation (e.g., Karhunen–Loève expansion)

$$a(\boldsymbol{x}, \boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j=1}^{\infty} y_j \, \psi_j(\boldsymbol{x}), \qquad \boldsymbol{x} \in D, \quad \boldsymbol{y} \in [-\tfrac{1}{2}, \tfrac{1}{2}]^{\mathbb{N}},$$

by sample variables y_j. Use in porous flow using Darcy's law:

$$q(\boldsymbol{x}, \boldsymbol{y}) + a(\boldsymbol{x}, \boldsymbol{y}) \nabla p(\boldsymbol{x}, \boldsymbol{y}) = f(\boldsymbol{x}),$$
$$\nabla \cdot q(\boldsymbol{x}, \boldsymbol{y}) = 0.$$

See, e.g., Barth, Charrier, Cliffe, Dick, Gantner, Giles, Graham, Haji-Ali, Harbrecht, Kuo, Le Gia, N., Nichols, Nobile, Peters, Robbe, Scheichl, Schwab, Siebenmorgen, Sloan, Teckentrup, Tempone, Ullmann, Vandewalle, Zollinger, von Schwerin, ...

Example: option pricing (d = hundreds, thousands, ∞)

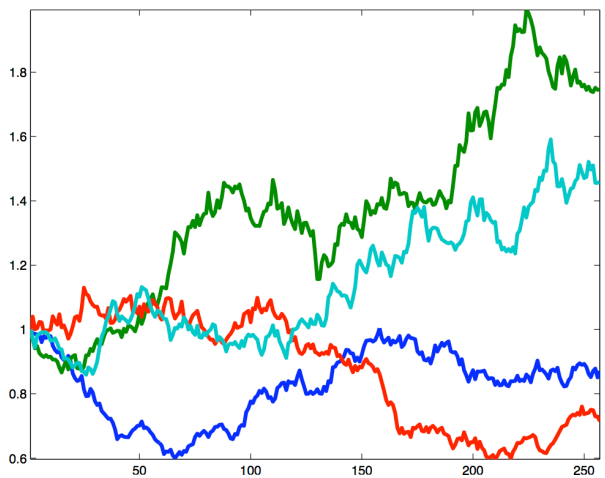
Simulation of SDE

$$\mathrm{d}X(t) = a(X(t))\,\mathrm{d}t + b(X(t))\,\mathrm{d}W(t), \quad X(0) = X_0, \quad 0 \le t \le T,$$

using Euler–Maruyama, $\widehat{X}_0 = X_0$,

$$\widehat{X}_{i+1} = \widehat{X}_i + a(\widehat{X}_i)\,h + b(\widehat{X}_i)\,\sqrt{h}\,Z_i, \quad i = 1, \ldots, n-1, \quad h = T/n,$$

with Z_i sampled from standard normal distribution.



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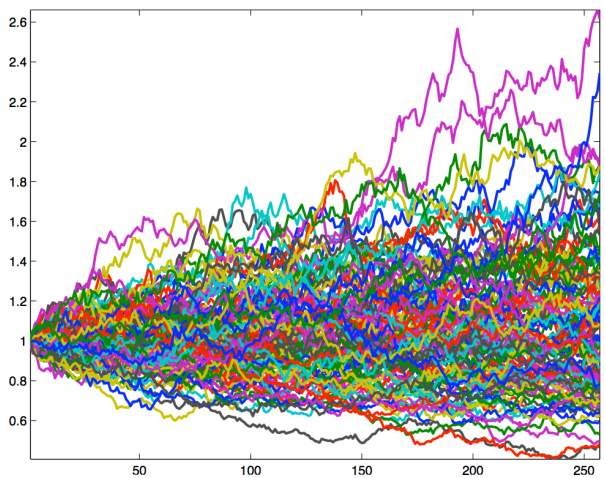

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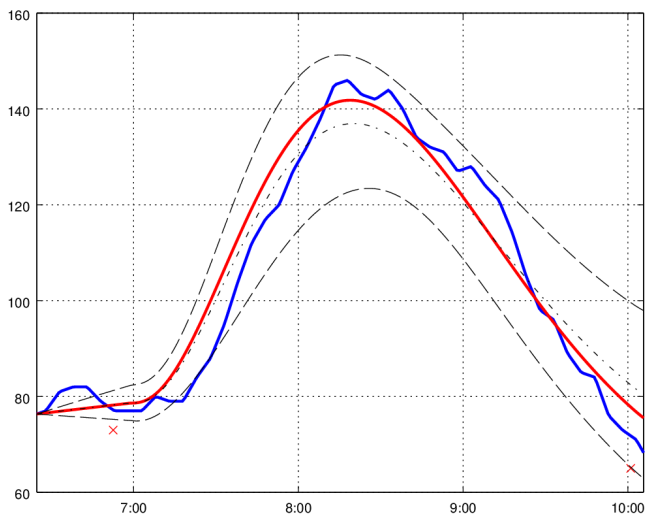
Example: Bayesian integrals (d = hundreds, thousands, ∞)

Simulation of insulin-glucose model

$$\mathrm{d}G(t)/\mathrm{d}t = -\lambda\big(G(t) - G_b\big) - \beta X(t) G(t) + R_a(t)$$
$$\mathrm{d}X(t)/\mathrm{d}t = -\mu X(t) + \mu\big(I(t) - I_b\big)$$

to infer parameters and quantify input uncertainty given noisy measurement $G^{\eta}_{\mathrm{ref}}(t)$ and uncertain input data $R_a(t)$.



Using evaluation of the integral point-of-view: see, e.g., Dick, Gantner, Le Gia, N., Scheichl, Schillings, Schwab, Stuart, Teckentrup, ...

Product rules

"The curse by construction"

What kind of cubature/quadrature method to use for d large?

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$$2^{100} = 1267650600228229401496703205376 \approx 10^{30}.$$

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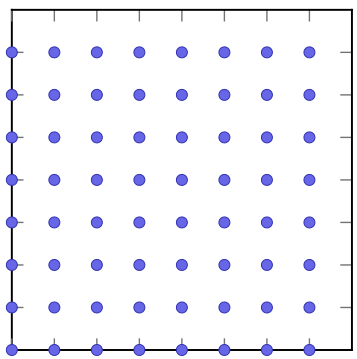
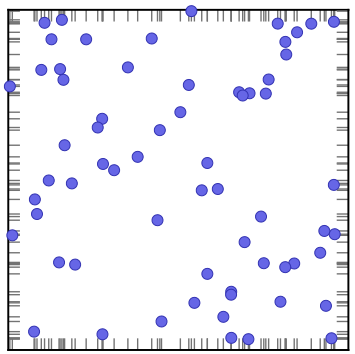
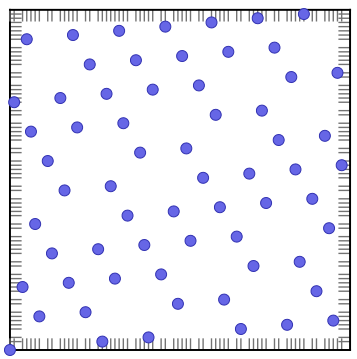
THE CURSE OF DIMENSIONALITY!

(Could try luck with "sparse" grid method; but not $d = 100$ out of the box, same issue.)
(An appropriate definition for the curse and intractability follows.)

Monte Carlo type methods: $\frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{x}_k)$

What kind of cubature/quadrature method to use for d large?

- A product of classical quadrature rules? 💣
  → $N = m^d$ ⇒ The curse "by construction"!
- The plain Monte Carlo method: $\boldsymbol{x}_k \sim U[0,1)^d$.
  → Free to choose N.
- Quasi-Monte Carlo methods: deterministic points using some algebraic structure.
  → Free to choose N.

grid	MC	QMC
		
$N = m^d$	N free	N free
error $= O(N^{-r/d})$	std $= O(N^{-1/2})$	error $= O(N^{-1}), \ldots$

Lattice rules rule! Lattice rules rule! Lattice rules rule!

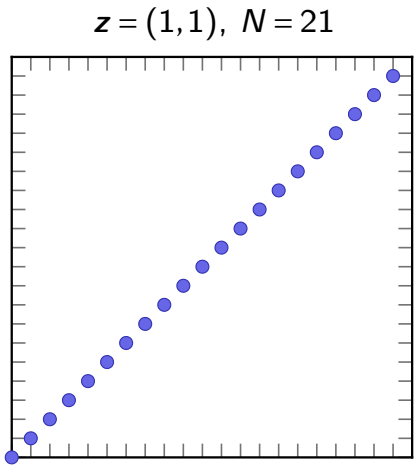
Rank-1 lattice rule: given N and integer generating vector $\boldsymbol{z}$:

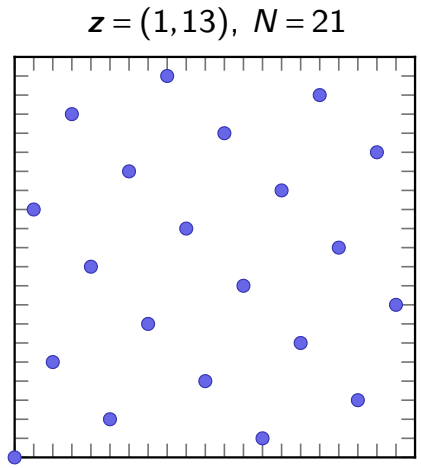
$$\boldsymbol{x}_k = \left\{ \frac{\boldsymbol{z}k}{N} \right\} := \frac{\boldsymbol{z}k}{N} \bmod 1 = \frac{\boldsymbol{z}k \bmod N}{N}, \qquad k = 0, \ldots, N-1.$$

Classical references: Niederreiter (1992), Sloan & Joe (1994).

"Good" lattice rules require "good" generating vectors $\boldsymbol{z} \in \mathbb{Z}^d$.

Obviously $\boldsymbol{z} = (1, \ldots, 1)$ will only have diagonal points in $[0,1]^d$.





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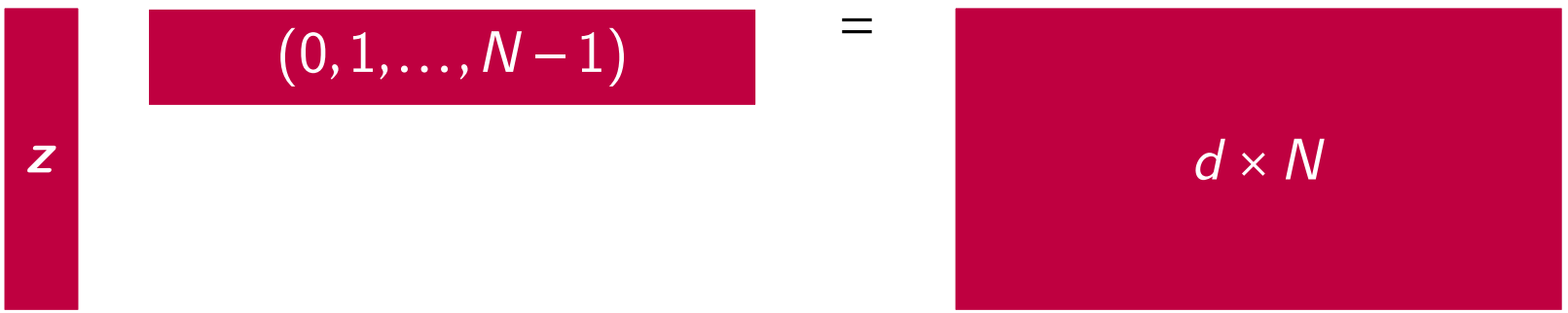
How to find "good" rules? (More later in the talk.)

→ 2D: Fibonacci lattice rules: $\boldsymbol{z} = (1, F_{k-1})$, $N = F_k$.

→ Component-by-component construction, see, e.g., Dick, Joe, Korobov, Kritzer, Kuo, N., Pillichshammer, Sloan, Suryanarayana, Weimar, ...

→ Fast component-by-component construction, see, e.g, Cools, Dick, Korobov, Kritzer, Laimer, Leobacher, Kuo, Le Gia, N., Matthysen, Pillichshammer, Schwab, ...

Visual mind-image (vectorization)



One-liners in Matlab/Octave, Python, ...

So assume you are given a "good" $\boldsymbol{z}$ for your choice of N, then

$$Q_N(f;\boldsymbol{z},N) = \frac{1}{N}\sum_{k=0}^{N-1} f\left(\frac{\boldsymbol{z}k \bmod N}{N}\right), \quad \text{and take eg } f(\boldsymbol{x}) = \left|\sum_{j=1}^{d} \mathrm{e}^{2\pi \mathrm{i} x_j}\right|^r.$$

(Example $I(f)$ is expected distance of rth moment of distance travelled by d-step random walk in the plane, see, Borwein, N., Straub, Wan (2011).)

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```
z = [1; 55]; N = 89; % points as [d x N] (Fortran), dim=1,2
f = @(r, x) abs( sum( exp(2*pi*1i*x), 1 ) ).^r;
% one-liner:
Q = mean( f(1, mod(z*(0:N-1), N)/N ) )
```

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```

```
from numpy import *; # using Numpy
z = [1, 55]; N = 89; # points as [N x d] (C), axis=0,1
f = lambda r, x: abs( sum( exp(2*pi*1j*x), axis=1 ) )**r
# one-liner:
Q = mean( f(1, (outer(range(N), z) % N)/float(N) ) )
```

Fixed N is boring, so, . . . , in come lattice sequences

- Let $\varphi_b(k)$ be the radical inverse function in base b:

$$\varphi_b : \mathbb{N}_0 \to [0,1) : (\cdots k_3 k_2 k_1 k_0)_b \mapsto (0.k_0 k_1 k_2 k_3 \cdots)_b.$$

- Hickernell & Niederreiter (2003), Hickernell, Hong, L'Écuyer, Lemieux (2000),

$$\boldsymbol{x}_k = \boldsymbol{z}\,\varphi_b(k) \bmod 1, \qquad k = 0,1,\ldots,$$

equivalently, for some m,

$$\boldsymbol{x}_k = (\boldsymbol{z}\,\mathrm{rev}_{b,m}(k) \bmod b^m)/b^m, \qquad k = 0,\ldots,b^m-1,$$

$\mathrm{rev}_{b,m}(k) = [\varphi_b(k) b^m]$ reverses the digits in an m-digit word.

→ Fast CBC construction of rules good for a range of m: Cools, Kuo, N. (2016), Dick, Pillichshammer, Waterhouse (2008).
→ For $b = 2$, bitreverse can be done in $\log_2(m)$ (bithacks).

An alternative sequence construction

- Typical trick to generate an $(s+1)$-dimensional digital net with b^m points from an s-dimensional sequence: add $x_0 = k/b^m$, $k = 0, \ldots, b^m - 1$, as the first dimension.

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- Idea from Korobov (1961): take s-dimensional lattice rule with $z_1 = 1$, drop first dimension to obtain $(s-1)$-dimensional lattice sequence. Ok for $O(N^{-1})$, see Hickernell, Kuo, Kritzer & N. (2011).

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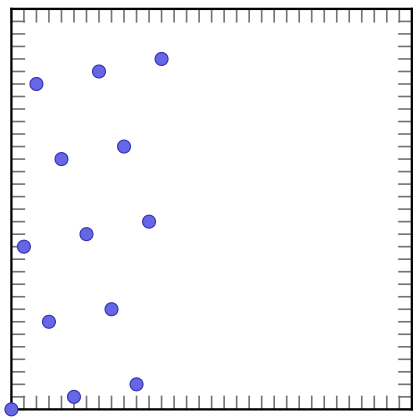
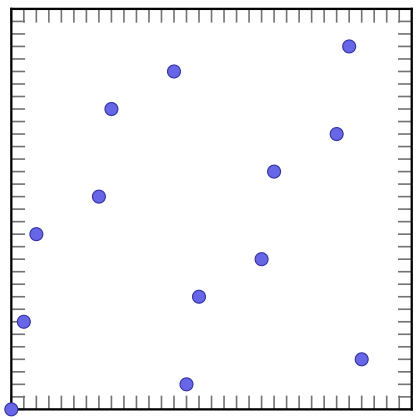
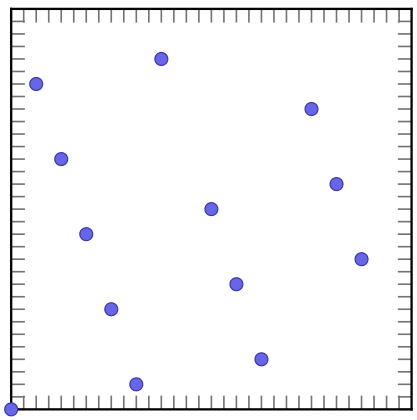
"First" 13 points of a base 2 lattice sequence optimized over $2^1,\dots,2^5$ with $z = (1,13,27,\dots)$:


Initial part of lattice


Korobov-seq


Radical-inverse-seq

Korobov trick for lattice sequence

```
% For a rule with z(1)=1 and length(z) >= d+1
acc = sum( f( mod( z(2:d+1) * (0:n1-1) , N ) / N )
Q1 = acc / n1
acc = acc + sum( f( mod( z(2:d+1) * (n1:n2-1) , N ) / N )
Q2 = acc / n2
...
```

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Q2 = acc / n2
...
```

Note: Although the above is a cool trick, we provide a Matlab/Octave point generator which can be used like `rand` and uses the radical-inverse method (using the bithacks bitreverse):

```
latticeseq_b2('init0', z, N);
acc = sum( f( latticeseq_b2(d, n1) )
Q1 = acc / n1
acc = acc + sum( f( latticeseq_b2(d, n2) )
Q2 = acc / n2
...
```

Randomly shifted lattice rules

To obtain an error estimator: take i.i.d. random shifts of the lattice

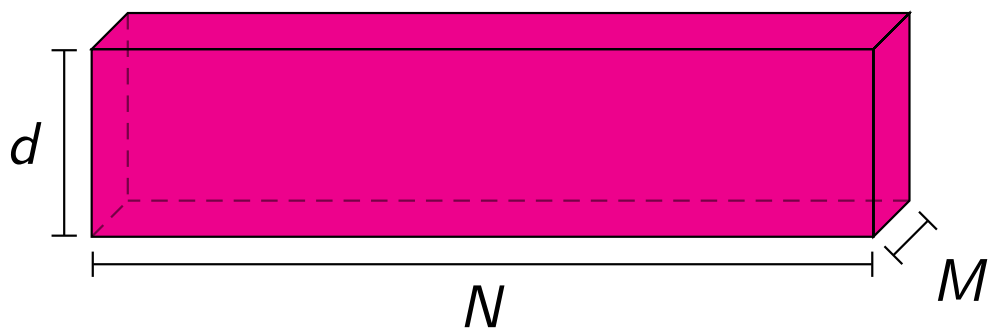
$$\boldsymbol{x}_k^{(i)} = \left(\boldsymbol{x}_k + \boldsymbol{\Delta}^{(i)}\right) \bmod 1 = \frac{\left(\boldsymbol{z}k + N\boldsymbol{\Delta}^{(i)}\right) \bmod N}{N}, \quad i = 1, \ldots, M,$$

to obtain M independent estimates $Q_N^{(1)}, \ldots, Q_N^{(M)}$. Then

$$\overline{Q}_{M\times N} = \frac{1}{M}\sum_{i=1}^{M} Q_N^{(i)}, \quad \mathrm{std}(\overline{Q}_{M\times N}(f)) = \frac{\mathrm{std}(Q_N^{(1)}, \ldots, Q_N^{(M)})}{\sqrt{M}}.$$

Singleton expansion in Matlab/Octave to generate the points $[d \times N \times M]$:

```
mod(bsxfun(@plus, reshape(z*(0:N-1), d, N, 1),
                  reshape(N*shifts, d, 1, M)), N) / N
```



How to measure deterministic algorithms?

- Worst-case error for approximating $I(f)$ by $Q_N(f)$ for $f \in \mathcal{F}_d$:

$$e(Q_N;\mathcal{F}_d) := \sup_{\substack{f\in\mathcal{F}_d \\ \|f\|_{\mathcal{F}_d}\le 1}} \big|I(f)-Q_N(f)\big| \le \text{upper bound for } Q_N.$$

(And the RMS expectation over random shifts in case of a randomly shifted rule.)

- Best possible error using N function values (benchmark):

$$e(N;\mathcal{F}_d) := \inf_{Q_N:\{(w_k,\boldsymbol{x}_k)\}_{k=1}^N} e(Q_N;\mathcal{F}_d) \ge \text{lower bound for any } Q_N$$

$$= \textit{error of best algorithm using } N \textit{ function evaluations}.$$

- Information complexity: the minimal number of function values needed to reach error at most ϵ:

$$n(\epsilon;\mathcal{F}_d) := \min\big\{N : \exists Q_N \text{ for which } e(Q_N;\mathcal{F}_d)\le\epsilon\big\}$$

$$= \textit{number of function evaluations of best algorithm}.$$

See a multitude of references, e.g., Novak (2016) or the Novak–Woźniakowski trilogy (2008,2010,2012), ...

The curse of dimensionality & types of tractability

Tractability started by Woźniakowski (1994) and since then vastly expanding...

- The curse of dimensionality is now defined as needing an exponential number of function values in d to reach an error $\epsilon \leq \epsilon_0$:

$$n(\epsilon; \mathscr{F}_d) \geq c\,(1+\gamma)^d, \qquad \text{for some } c, \gamma, \epsilon_0 > 0.$$

- A problem is called (weakly) tractable if

$$\lim_{\epsilon^{-1}+d \to \infty} \frac{\ln n(\epsilon, d)}{\epsilon^{-1} + d} = 0,$$

  and intractable otherwise.
- Different types, e.g., polynomial tractability

$$n(\epsilon; \mathscr{F}_d) \leq c\,\epsilon^{-p}\,d^q, \qquad \text{for some } c, p, q \geq 0.$$

See a multitude of references, in particular the Novak–Woźniakowski trilogy (2008,2010,2012), ...

The curse might always be there...

Assume $f \in \mathscr{F}_d$ when

$$\|f\|_{\mathscr{F}_d} := \max_{\boldsymbol{x},\boldsymbol{y}\in[0,1]^d} \frac{|f(\boldsymbol{x})-f(\boldsymbol{y})|}{\|\boldsymbol{x}-\boldsymbol{y}\|_\infty} \quad < \quad \infty,$$

then (Maung Zho Newn and Sharygin, 1971)

$$e(N,\mathscr{F}_d) = \frac{d}{2d+2} N^{-1/d}.$$

See Novak's (2016) review in MCQMC2014:

Not just avoid the "curse by construction", but also

- rate independent of d $\Rightarrow$ "mixed dominating smoothness".
- constant $C_{d,\alpha}$ independent of d $\Rightarrow$ "weighted spaces".

Aims

- **Mixed dominating smoothness spaces:** Move from typical Sobolev norm with $\|D^{\boldsymbol{\tau}} f\|$ bounded for $\tau_1 + \cdots + \tau_d \leq \alpha$, which gives $O(N^{-\alpha/d})$ to $(\tau_1, \ldots, \tau_d) \leq \alpha$ which gives $\sim O(N^{-\alpha})$.
- **Dimension-independent error bounds:** Switch to weighted spaces: not all combinations of variables are as important. Denote the importance of the variables in $\mathfrak{u} \subseteq \{1, \ldots, d\}$ by $\gamma_{\mathfrak{u}}$.

Mixed dominating smoothness: Novak, Sickel, Temlyakov, Ullrich ×2, ...
Weights: Hickernell (1998), Sloan & Woźniakowski (1998), Novak–Woźniakowski trilogy (2008,2010,2012), ...

Spaces based on series representations & Koksma–Hlawka

Assume an L_2-ONB $\{\phi_h\}_h$, with $\phi_0 = 1$, $Q_N(1) = 1$, and abs. summ.

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h}} \widehat{f}(\boldsymbol{h})\,\phi_{\boldsymbol{h}}(\boldsymbol{x}), \qquad \text{with} \quad \widehat{f}(\boldsymbol{h}) := \int_{[0,1]^d} f(\boldsymbol{x})\,\overline{\phi_{\boldsymbol{h}}(\boldsymbol{x})}\,\mathrm{d}\boldsymbol{x},$$

Spaces based on series representations & Koksma–Hlawka

Assume an L_2-ONB $\{\phi_{\boldsymbol{h}}\}_{\boldsymbol{h}}$, with $\phi_0 = 1$, $Q_N(1) = 1$, and abs. summ.

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then, for $r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h}) > 0$ an "increasing" function,

$$\begin{aligned} \big|I(f) - Q_N(f)\big| &= \left|\sum_{\boldsymbol{h}\neq\boldsymbol{0}} \widehat{f}(\boldsymbol{h})\, Q_N(\phi_{\boldsymbol{h}})\, r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h})\, r_{\alpha,\boldsymbol{\gamma}}^{-1}(\boldsymbol{h})\right| \\ &\le \left(\sum_{\boldsymbol{h}} \big|\widehat{f}(\boldsymbol{h})\big|^p\, r_{\alpha,\boldsymbol{\gamma}}^{p}(\boldsymbol{h})\right)^{1/p} \left(\sum_{\boldsymbol{h}\neq\boldsymbol{0}} \big|Q_N(\phi_{\boldsymbol{h}})\big|^q\, r_{\alpha,\boldsymbol{\gamma}}^{-q}(\boldsymbol{h})\right)^{1/q} \\ &\qquad\qquad \text{norm} \qquad\qquad \times \qquad\qquad \text{worst-case error}. \end{aligned}$$

For $1 < p \le \infty$ and nice choices of $\phi_{\boldsymbol{h}}$, Q_N and $r_{\alpha,\boldsymbol{\gamma}}$ we can find a "worst-case" representer $\xi(\boldsymbol{x})$ for which

$$\big|Q_N(\xi) - I(\xi)\big|^{1/q} = e(Q_N, \mathscr{F}_d),$$

independent of the particular Q_N, e.g., Fourier series and lattice rules, Walsh series and digital nets, see N. (2014) and Hickernell (1998a,b).

Choice I

So we have (Let $\mathfrak{u}(\boldsymbol{h})$ be the support of $\boldsymbol{h}$.)

- choice of $r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h})$, controls the (decaying) importance of $\phi_{\boldsymbol{h}}$:
  - polynomial decay, e.g., $r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h}) = \gamma_{\mathfrak{u}(\boldsymbol{h})} \prod_{j=1}^{d} (1+h_j)^{\alpha}$,
  - exponential decay, e.g., $r_{\boldsymbol{a},\boldsymbol{b},\boldsymbol{\gamma}}(\boldsymbol{h}) = \gamma_{\mathfrak{u}(\boldsymbol{h})} \prod_{j=1}^{d} \exp(a_j h_j^{b_j})$,
- choice of $\boldsymbol{\gamma} = \{\gamma_{\mathfrak{u}}\}_{\mathfrak{u} \subseteq \{1,\ldots,d\}}$:
  - product weights: $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_{\{j\}}$,
  - order-dependent weights: $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}$,
  - POD weights: $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_{\{j\}}$,
  - ...,
- choice of $\phi_{\boldsymbol{h}}$,
- choice of Q_N, i.e., $\{(w_k, \boldsymbol{x}_k)\}_{k=1}^{N}$.

Weights: Sloan, Woźniakowski (1998), Dick, Sloan, Wang, Woźniakowski (2004), Kuo, Schwab, Sloan (2012), Dick, Kuo, Le Gia, N., Schwab (2014), ...
Cos: Dick, N., Pillichshammer (2013), Suryanarayana, N., Cools (2015), Potts, Volkmer (2015), Cools, Kuo, N., Suryanarayana (2016), ...
Exp: Dick, Larcher, Pillichshammer, Woźniakowski (2011), Kritzer, Pillichshammer, Woźniakowski (2014), Irrgeher, Kritzer, Leobacher, Pillichshammer. (2015), Nguyen, N. (201x), Nguyen, N., Cools (201y), ...

Choice II

So we have

- choice of $r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h})$, controls the (decaying) importance of $\phi_{\boldsymbol{h}}$,
- choice of $\boldsymbol{\gamma} = \{\gamma_{\mathfrak{u}}\}_{\mathfrak{u}\subseteq\{1,\ldots,d\}}$,
- choice of $\phi_{\boldsymbol{h}}$:
  - Fourier basis,
  - Walsh basis,
  - Cosine basis,
- choice of Q_N, i.e., $\{(w_k, \boldsymbol{x}_k)\}_{k=1}^N$:
  - Lattice rules/sequences,
  - Digital nets/sequences, polynomial lattice rules,
  - Tent-transformed lattice rules/sequences.

Weights: Sloan, Woźniakowski (1998), Dick, Sloan, Wang, Woźniakowski (2004), Kuo, Schwab, Sloan (2012), Dick, Kuo, Le Gia, N., Schwab (2014), ...
Cos: Dick, N., Pillichshammer (2013), Suryanarayana, N., Cools (2015), Potts, Volkmer (2015), Cools, Kuo, N., Suryanarayana (2016), ...
Exp: Dick, Larcher, Pillichshammer, Woźniakowski (2011), Kritzer, Pillichshammer, Woźniakowski (2014), Irrgeher, Kritzer, Leobacher, Pillichshammer. (2015), Nguyen, N. (201x), Nguyen, N., Cools (201y), ...

Reproducing kernel Hilbert spaces, $p = q = 2$

Given a one-dimensional reproducing kernel $K(x,y) = \overline{K(y,x)}$.
Suppose $\mathscr{H}(K)$ is separable: $\mathscr{H}(K) = \operatorname{span}\{\phi_h\}_h$ and $\phi_0 = 1$.
Determine the eigenvalues and eigenfunctions, and assume $\lambda_0 = 1$,

$$\int_{[0,1]} \phi(x)\,\overline{K(x,y)}\,\mathrm{d}x = \lambda\,\phi(y).$$

Then

$$K(x,y) = \sum_h \frac{\phi_h(x)}{\sqrt{\lambda_h}}\,\frac{\overline{\phi_h(y)}}{\sqrt{\lambda_h}} = \sum_h \frac{\phi_h(x)}{\|\phi_h\|_{L_2}}\,\frac{\overline{\phi_h(y)}}{\|\phi_h\|_{L_2}},$$

the ϕ_h are L_2-orthogonal, with $\|\phi_h\|_{L_2} = \sqrt{\lambda_h}$ and $\|\phi_h\|_{\mathscr{H}} = 1$, with

$$\langle f,g\rangle_{\mathscr{H}} = \sum_h \lambda_h\,\widehat{f}(h)\,\overline{\widehat{g}(h)}, \qquad \|f\|^2_{\mathscr{H}} = \sum_h \lambda_h\,\bigl|\widehat{f}(h)\bigr|^2.$$

Multivariate weighted reproducing kernel Hilbert space

Use the one-dimensional space as building block for d dimensions by taking weighted tensor products (tensor product basis):

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1,\dots,d\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} K(x_j,y_j) = \sum_{\boldsymbol{h}} \gamma_{\mathfrak{u}(\boldsymbol{h})} \prod_{j=1}^{d} \frac{\phi_{h_j}(x_j)}{\sqrt{\lambda_{h_j}}} \frac{\overline{\phi_{h_j}(y_j)}}{\sqrt{\lambda_{h_j}}}$$

$$= \sum_{\boldsymbol{h}} r^{-2}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h})\, \phi_{\boldsymbol{h}}(\boldsymbol{x})\, \overline{\phi_{\boldsymbol{h}}(\boldsymbol{y})},$$

with

(You could now interpret α as the decay of the eigenvalues.)

$$r^{-2}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h}) = \gamma_{\mathfrak{u}(\boldsymbol{h})} \prod_{j\in\mathfrak{u}} \lambda_{h_j}^{-1} = \gamma_{\mathfrak{u}(\boldsymbol{h})} \prod_{j=1}^{d} \lambda_{h_j}^{-1},$$

and $\mathfrak{u}(\boldsymbol{h}) = \{h_j : h_j \neq 0\}$ the support of $\boldsymbol{h}$. Now, $\gamma_\emptyset = 1$, $Q_N(1) = 1$,

$$e^2(Q_N;\mathscr{H}) = -1 + \sum_{k,\ell=1}^{N} w_k\, w_\ell\, K(\boldsymbol{x}_k,\boldsymbol{y}_\ell).$$

Korobov type spaces $\mathscr{E}_{\alpha,p}$: Lattice rules

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h}\in\mathbb{Z}^d} \widehat{f}(\boldsymbol{h}) \exp(2\pi \mathrm{i}\, \boldsymbol{h}\cdot\boldsymbol{x}), \quad \|f\|^p_{\mathscr{E}_{\alpha,p}} := \sum_{\boldsymbol{h}\in\mathbb{Z}^d} \left|\widehat{f}(\boldsymbol{h})\right|^p r^p_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h}) < \infty.$$

Traditional choice of r, for $\alpha > 1/q$:

$$r^p_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{h}) = \gamma^{-1}_{\mathfrak{u}(\boldsymbol{h})} \prod_{j=1}^{d} r^p_\alpha(h_j), \qquad r^p_\alpha(h_j) = \max(1, |h_j|^{p\alpha}).$$

- Unweighted ⇒ intractable. Sloan & Woźniakowski (2001).
- Strong tractability with product weights iff $\sum_{j\geq 1} \gamma_{\{j\}} < \infty$. Ditto.
- CBC construction of lattice rule achieving optimal $O(N^{-\alpha+\delta})$, $\delta > 0$, if $\sum_{j\geq 1} \gamma_{\{j\}}^{1/(2\alpha)} < \infty$ with constant independent of d for product weights. Kuo (2003).
- Unweighted strong tractability for sufficient large α and e.g. $r^2_\alpha(h_j) = (2\pi h)^{2\alpha}$, i.e., periodic Sobolev space, under the condition of permutation-invariance, e.g. $f(x_1, x_2) = f(x_2, x_1)$. N., Suryanarayana, Weimar (2015,201z).
- Several results on exponential convergence: Dick, Larcher, Pillichshammer, Woźniakowski (2011), Kritzer, Pillichshammer, Woźniakowski (2014), Irrgeher, Kritzer, Leobacher, Pillichshammer. (2015), Nguyen, N. (201x), Nguyen, N., Cools (201y), ...

Cosine space $\mathscr{C}_{\alpha,p}$: Tent-transformed lattice rules

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h}\in\mathbb{N}_0^d} \widehat{f}_{\cos}(\boldsymbol{h}) \prod_{\substack{j=1\\ h_j\neq 0}}^{d} \sqrt{2}\cos(\pi h_j x_j), \quad \|f\|_{\mathscr{C}_{\alpha,p}}^p := \sum_{\boldsymbol{h}\in\mathbb{N}_0^d} \left|\widehat{f}_{\cos}(\boldsymbol{h})\right|^p r_{\alpha,\boldsymbol{\gamma}}^p(\boldsymbol{h}).$$

In the Hilbert case, for $\alpha = 1$ and $d = 1$:

$$\langle f, g\rangle_{\mathscr{C}_{1,2}} = \left(\int_0^1 f(x)\,\mathrm{d}x\right)\left(\int_0^1 g(x)\,\mathrm{d}x\right) + \frac{(2\pi)^2}{\gamma}\int_0^1 f'(x)\,g'(x)\,\mathrm{d}x.$$

For $\gamma = (2\pi)^2$ this is the inner product of the unanchored Sobolev space $\mathscr{W}_{1,2}$, Dick, N., Pillichshammer (2013).

- This gives deterministic $O(N^{-1})$ for tent-transformed lattice rules in $\mathscr{W}_{1,2}$. Tent-transform: elementwise $x \mapsto 1 - |2x-1|$.
- Same tractability results as for Korobov space.
- Thus for product weights, optimal dimension-independent $O(N^{-\alpha+\delta})$, $\delta > 0$, if $\sum_{j\geq 1} \gamma_{\{j\}}^{1/(2\alpha)} < \infty$.

Sobolev spaces and Walsh spaces

- Unanchored Sobolev space $\mathcal{W}_{\alpha,p}$ of order $\alpha = 1$:
  - randomly shifted lattice rules/sequences, or
  - (deterministic) tent-transformed lattice rules/sequences.
- Walsh spaces based on Walsh expansion of function:
  - digital nets/sequences,
  - polynomial lattice rules.
- Higher order Sobolev spaces embedded in Walsh spaces:
  - higher order polynomial lattice rules,
  - interlaced digital nets/sequences,
  - interlaced polynomial lattice rules.

See, e.g., Hickernell (2002), Dick & Pillichshammer (2009), Baldeaux, Dick, Leobacher, N., Pillichshammer (2012), Dick, Kuo, Le Gia, N., Schwab (2014), ...

Polynomial lattice rules ≡ lattice rules over finite field

For $x \in [0,1)$ identify (uniquely) (Let's fix the base of the finite field to $b = 2$.)

$$x = \sum_{i \geq 1} x_i 2^{-i} \simeq (x_1 x_2 \cdots)_2 \simeq x_1 \chi^1 + x_2 \chi^2 + \cdots = x(\chi).$$

Likewise for $k \in \mathbb{N}_0$

$$k = \sum_{i \geq 0} k_i 2^i \simeq (\cdots k_2 k_1 k_0)_2 \simeq k_0 \chi^0 + k_1 \chi^1 + \cdots = k(\chi).$$

For a polynomial $P(\chi)$ over $\mathbb{Z}_2$ with $\deg(P) = n$ define the polynomial lattice points

$$\boldsymbol{x}_k(\chi) = \frac{\boldsymbol{z}(\chi) k(\chi) \bmod P(\chi)}{P(\chi)} \quad \text{over } \mathbb{Z}_2[\chi], \quad \text{for } k = 0, \ldots, b^m - 1.$$

The points in the unit cube $[0,1)^d$ are obtained by evaluating each $x(\chi)$ in $\chi = b = 2$ (up to χ^{-n}, or further).

Recap: Lattice rules

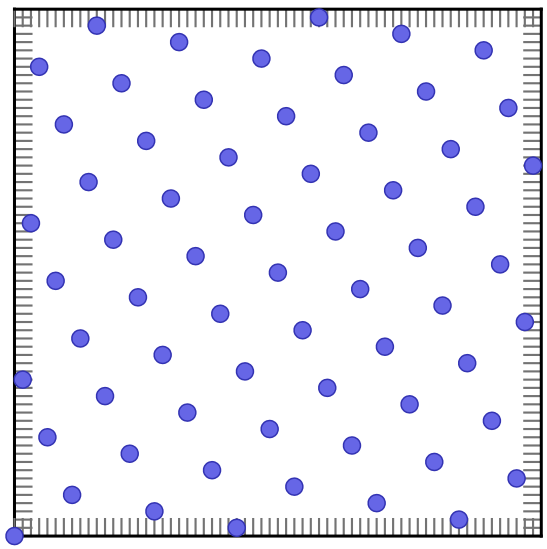
For a generating vector $\boldsymbol{z} \in \mathbb{Z}_N^d$:

$$\boldsymbol{x}_k = \frac{\boldsymbol{z}k \bmod N}{N}, \qquad \text{for } 0 \le k < N.$$

Then

$$Q_N(f; \boldsymbol{z}, N) = \frac{1}{N} \sum_{k=0}^{N-1} f(\boldsymbol{x}_k).$$

Components of z_j relatively prime to N:
then z_j defines a permutation for dimension j.



Polynomial lattice rules

For a generating vector $\boldsymbol{z}(\chi) \in (\mathbb{Z}_2[\chi]/P(\chi))^d$:

$$\boldsymbol{x}_k(\chi) = \frac{\boldsymbol{z}(\chi)k(\chi) \bmod P(\chi)}{P(\chi)}, \qquad \text{for } \deg(k(\chi)) < 2^m.$$

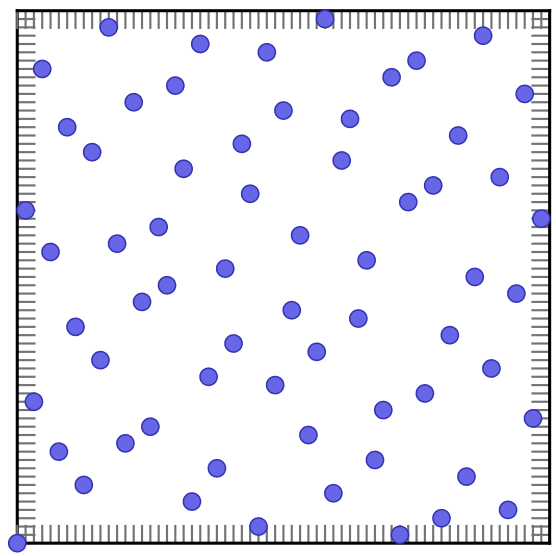
Then

$$Q_N(f; \boldsymbol{z}(\chi), P(\chi)) = \frac{1}{N} \sum_{k=0}^{2^m-1} f(\boldsymbol{x}_k(\chi)|_{\chi=2}).$$

If $z_j(\chi)$ relatively prime to $P(\chi)$:
then $z_j(\chi)$ defines a permutation for dim j.

→ Typically, take $P(\chi)$ irreducible over $\mathbb{Z}_2[\chi]$.

Niederreiter (1992), Dick & Pillichshammer (2009),
Lemieux & L'Écuyer (2002), ...



Digital net formulation

Assembling the n bits of each component of $\boldsymbol{x}_k$ in a vector $\vec{x}_{k,j}$, and the m bits of k in a vector $\vec{k}$, this is equivalent to

$$\vec{x}_{k,j} = C_j \vec{k} \qquad \text{over } \mathbb{Z}_2$$

where $C_j \in \mathbb{Z}_2^{n \times m}$ is a Hankel matrix formed by the recursion of $z_j(\chi)/P(\chi)$ over $\mathbb{Z}_2$. I.e., for each dimension j, we have

$$\begin{pmatrix} x_{k,j,1} \\ x_{k,j,2} \\ x_{k,j,3} \\ \vdots \\ x_{k,j,n} \end{pmatrix} = \begin{pmatrix} & & \\ \vec{c}_{j,1} & \cdots & \vec{c}_{j,m} \\ & & \end{pmatrix} \begin{pmatrix} k_0 \\ k_1 \\ \vdots \\ k_{m-1} \end{pmatrix} = \bigoplus_{\substack{i=0 \\ k_i \neq 0}}^{m-1} \vec{c}_{j,i},$$

where $\oplus$ is addition over $\mathbb{Z}_2$.
$\rightarrow$ "In parallel" on n bits this is the `xor` operation...

Representation

By the same representation of integers and vectors over $\mathbb{Z}_2$:

$$C_j = \begin{pmatrix} \vec{c}_{j,1} & \cdots & \vec{c}_{j,m} \end{pmatrix} \in \mathbb{Z}_2^{n \times m} \quad \simeq \quad \begin{pmatrix} c_{j,1} & \cdots & c_{j,m} \end{pmatrix} \in \mathbb{Z}^m.$$

Inverse: Print generating matrices given as integers $\mathtt{C} = (C_{j,i})$, $j = 1, \ldots, d$, $i = 1, \ldots, m$:

```
n = max(floor(log2(C(:)))+1); [d, m] = size(C);
permute(reshape(rot90(dec2bin(C, n)-'0'), n, d, m),[1 3 2])
```

- Each matrix $C_j \in \mathbb{Z}_2^{n \times m}$ is represented as m integers.
- Integers need to have at least $\geq n$ bits.
- Use top row as least significant bit.
- Running through k in Gray code ordering only changes one bit.
- Next point: `xor` "state" with column of changed bit.

Interlaced points

Given a digital net in base b with $s = \alpha d$ dimensions:

$$\boldsymbol{x}_k = \begin{pmatrix} x_{k,1} \\ x_{k,2} \\ \vdots \\ x_{k,\alpha} \\ \hline x_{k,\alpha+1} \\ \vdots \\ x_{k,2\alpha} \\ \hline \vdots \\ x_{k,\alpha d} \end{pmatrix} = \begin{pmatrix} 0.x_{k,1,1}\, x_{k,1,2}\, x_{k,1,3} \cdots x_{k,1,m} \\ 0.x_{k,2,1}\, x_{k,2,2}\, x_{k,2,3} \cdots x_{k,2,m} \\ \vdots \\ 0.x_{k,\alpha,1}\, x_{k,\alpha,2}\, x_{k,\alpha,3} \cdots x_{k,\alpha,m} \\ \hline 0.x_{k,\alpha+1,1}\, x_{k,\alpha+1,2}\, x_{k,\alpha+1,3} \cdots x_{k,\alpha+1,m} \\ \vdots \\ 0.x_{k,2\alpha,1}\, x_{k,2\alpha,2}\, x_{k,2\alpha,3} \cdots x_{k,2\alpha,m} \\ \hline \vdots \\ 0.x_{k,\alpha d,1}\, x_{k,\alpha d,2}\, x_{k,\alpha d,3} \cdots x_{k,\alpha d,m} \end{pmatrix}$$

gives d dimensions with αm digits

$$y_{k,1} = 0.x_{k,1,1}\, x_{k,2,1} \cdots x_{k,\alpha,1} | x_{k,1,2}\, x_{k,2,2} \cdots x_{k,\alpha,2} | \cdots,$$

and so on...

See, e.g., Dick (2007), Dick & Goda (2013), ...

Interlaced points

Given a digital net in base b with $s = \alpha d$ dimensions:

$$\boldsymbol{x}_k = \begin{pmatrix} x_{k,1} \\ x_{k,2} \\ \vdots \\ x_{k,\alpha} \\ \hline x_{k,\alpha+1} \\ \vdots \\ x_{k,2\alpha} \\ \hline \vdots \\ x_{k,\alpha d} \end{pmatrix} = \begin{pmatrix} 0.x_{k,1,1}\, x_{k,1,2}\, x_{k,1,3} \cdots x_{k,1,m} \\ 0.x_{k,2,1}\, x_{k,2,2}\, x_{k,2,3} \cdots x_{k,2,m} \\ \vdots \\ 0.x_{k,\alpha,1}\, x_{k,\alpha,2}\, x_{k,\alpha,3} \cdots x_{k,\alpha,m} \\ \hline 0.x_{k,\alpha+1,1}\, x_{k,\alpha+1,2}\, x_{k,\alpha+1,3} \cdots x_{k,\alpha+1,m} \\ \vdots \\ 0.x_{k,2\alpha,1}\, x_{k,2\alpha,2}\, x_{k,2\alpha,3} \cdots x_{k,2\alpha,m} \\ \hline \vdots \\ 0.x_{k,\alpha d,1}\, x_{k,\alpha d,2}\, x_{k,\alpha d,3} \cdots x_{k,\alpha d,m} \end{pmatrix}$$

gives d dimensions with αm digits

$$y_{k,1} = 0.x_{k,1,1}\, x_{k,2,1} \cdots x_{k,\alpha,1} | x_{k,1,2}\, x_{k,2,2} \cdots x_{k,\alpha,2} | \cdots,$$

and so on...

See, e.g., Dick (2007), Dick & Goda (2013), ...

Interlaced points

Given a digital net in base b with $s = \alpha d$ dimensions:

$$\boldsymbol{x}_k = \begin{pmatrix} x_{k,1} \\ x_{k,2} \\ \vdots \\ x_{k,\alpha} \\ \hline x_{k,\alpha+1} \\ \vdots \\ x_{k,2\alpha} \\ \hline \vdots \\ x_{k,\alpha d} \end{pmatrix} = \begin{pmatrix} 0.x_{k,1,1}\, x_{k,1,2}\, x_{k,1,3} \cdots x_{k,1,m} \\ 0.x_{k,2,1}\, x_{k,2,2}\, x_{k,2,3} \cdots x_{k,2,m} \\ \vdots \\ 0.x_{k,\alpha,1}\, x_{k,\alpha,2}\, x_{k,\alpha,3} \cdots x_{k,\alpha,m} \\ \hline 0.x_{k,\alpha+1,1}\, x_{k,\alpha+1,2}\, x_{k,\alpha+1,3} \cdots x_{k,\alpha+1,m} \\ \vdots \\ 0.x_{k,2\alpha,1}\, x_{k,2\alpha,2}\, x_{k,2\alpha,3} \cdots x_{k,2\alpha,m} \\ \hline \vdots \\ 0.x_{k,\alpha d,1}\, x_{k,\alpha d,2}\, x_{k,\alpha d,3} \cdots x_{k,\alpha d,m} \end{pmatrix}$$

gives d dimensions with αm digits

$$y_{k,1} = 0.x_{k,1,1}\, x_{k,2,1} \cdots x_{k,\alpha,1} | x_{k,1,2}\, x_{k,2,2} \cdots x_{k,\alpha,2} | \cdots,$$

and so on...

See, e.g., Dick (2007), Dick & Goda (2013), ...

Generate the points

- Generate points in Gray code ordering.
- Only one integer (column) needs to be `xor`'d.
- Need to know which bit changed...

de Bruijn sequence for bit change:

```
db = [0, 1, 28, 2, 29, 14, 24, 3, 30, 22, 20, 15, 25, 17, 4, 8,
      31, 27, 13, 23, 21, 19, 16, 7, 26, 12, 18, 6, 11, 5, 10, 9];
jc = @(v) db( bitshift (mod(double(bitand(int32(v),-int32(v)))*0x077CB531,
                pow2(32)),-27)+1)+1; % mind the double because of Matlab madne
```

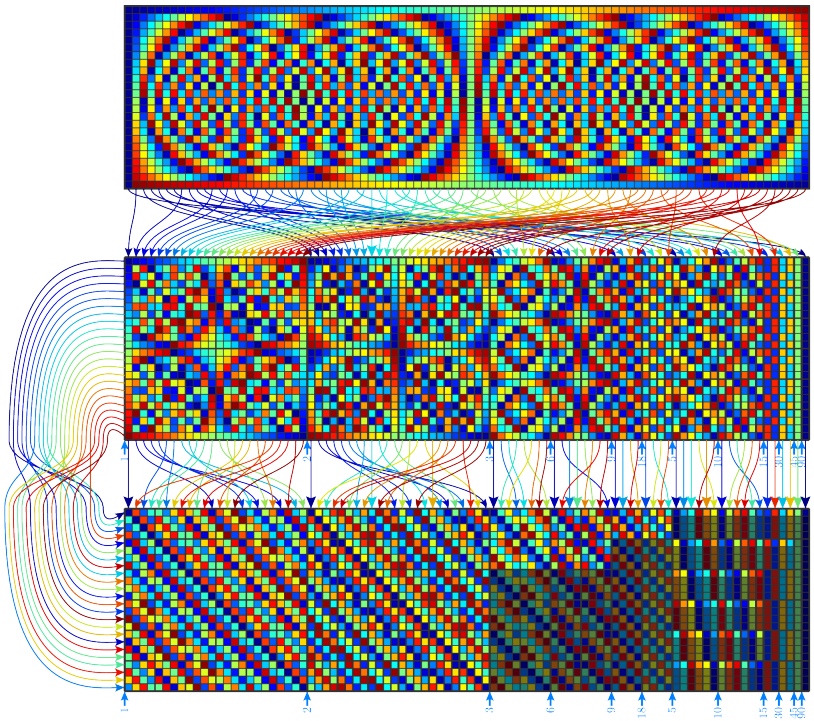
Generate points (for the fun of it):

```
k = 1:pow2(m)-1; K = numel(k);
P = reshape(reshape(mod(cumsum(
        reshape( fliplr (dec2bin(C(:,jc(k)),n)-'0'),d,K,n), 2), 2),
        d*K, n) * pow2(-1:-1:-n)', d, K);
```

→ Don't be silly: use `digitalseq_b2g` instead.

Construction of lattice rules and polynomial lattice rules

Point sets constructed for weighted spaces using fast component-by-component constructions using number theoretic transforms.



See https://www.cs.kuleuven.be/~dirkn/qmc4pde/ and https://www.cs.kuleuven.be/~dirkn/fast-cbc/.

See, e.g., N. & Cools (2006a,2006b), Cools, Kuo, & N. (2006), Dick, Kuo, Le Gia, N. & Schwab (2014), N. (2014), Kuo & N. (2016), ...
Variations and speedups by: Gantner, Kritzer, Laimer, Leobacher, Pillichshammer, Schwab, ...

Point generators

- Matlab/Octave: procedural generators like Matlab's `rand`:
  - `latticeseq_b2.m`: radical inverse lattice sequence generator,
  - `digitalseq_b2g.m`: gray coded radical inverse digital sequence generator (incl. higher-order, max 53 bit).
- Python: iterator classes, which can be used as standalone point generators from the command line (`__main__`):
  - `latticeseq_b2.py`: iterator based (`__iter__`), `set_state` for parallel computing,
  - `digitalseq_b2g.py`: ditto, arbitrary precision using `mpmath` if needed.
- C++: header file based implementation with driver program for the command line:
  - `latticeseq_b2.(h|cpp)`: complies to `ForwardIterator` concept, `set_state` for parallel computing,
  - `digitalseq_b2g.(h|cpp)`: ditto, max 64 bit.

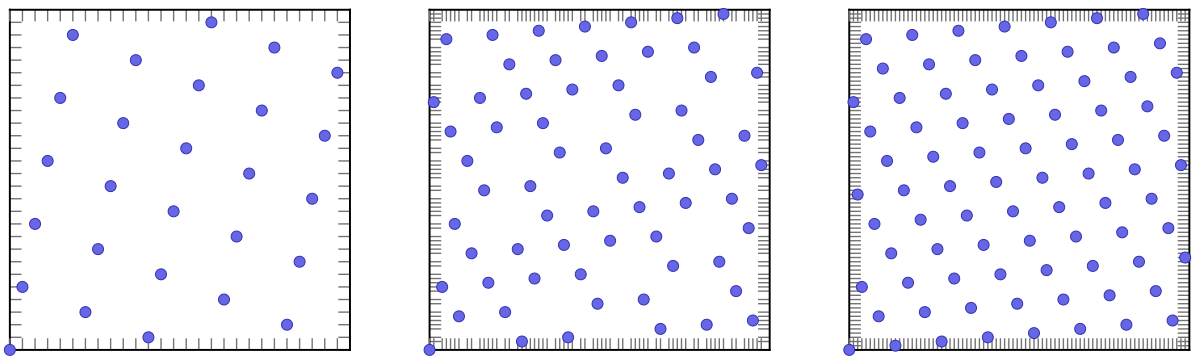
See https://www.cs.kuleuven.be/~dirkn/qmc4pde/ and https://www.cs.kuleuven.be/~dirkn/qmc-generators/.

Welcome to The Magic Point Shop!

Different flavours of quasi-Monte Carlo points to choose:

- Lattice rules.
- Lattice sequences.
- Polynomial lattice rules.
- Interlaced Sobol' sequences (higher-order).
- Interlaced polynomial lattice rules (higher-order).
- Interlaced Niederreiter–Xing sequence (higher-order).

And code (C++ and Matlab) to use them...



Subsidiaries: QMC4PDE: construct points for parametrised PDEs.

Bounds on derivatives

Assume bounds on derivatives of f, $\nu \in \{0,\ldots,\alpha\}^d$, up to $|\nu| = \sum_{j=1}^{s} \nu_j \leq \alpha$

$$\left\|(\partial^{\nu} f)(x_1,\ldots,x_d)\right\|_{\infty} = O\Big((|\nu + a_1|!)^{d_1} \prod_{j=1}^{d} (a_2\,\beta_j)^{\nu_j}\Big).$$

"SPOD-type" (smoothness-driven product and order dependent decay) and "POD-type" (product and order dependent decay, $\alpha = 1$) — coming from PDE context, see, e.g., Dick, Kuo, Le Gia, N., Schwab (2014), Kuo & N. (2016).

With e.g.

$$\beta_j = c\, j^{-d_2}$$

for some $d_2 > d_1 \geq 0$ and $c > 0$.
The parameter d_2 is the "decay".

Construction of specialized (polynomial) lattice rules

Lattice rules:

- randomly shifted lattice rules on $[0,1]^s$
  $\rightarrow$ randomly shifted Sobolev space W_1: $O(N^{-1})$
- randomly shifted lattice rules constructed for $\mathbb{R}^s$
  $\rightarrow$ "unbounded integrand space": $O(N^{-1})$
- tent-transformed lattice rules
  $\rightarrow$ Sobolev space W_1: $O(N^{-1})$

Digital nets:

- randomly shifted polynomial lattice rules
  $\rightarrow$ randomly shifted Sobolev space: $O(N^{-1})$
- higher order polynomial lattice rules
  $\rightarrow$ Sobolev space W_r embedded in ho Walsh space: $O(N^{-r})$
- higher order interlaced polynomial lattice rules
  $\rightarrow$ Sobolev space W_r embedded in ho Walsh space: $O(N^{-r})$

Take home message

- You can use QMC!
- It's easy!
- You are not afraid of the function spaces!
- You gladly found out about higher-order convergence $N^{-\alpha}$!
- You are happily finding online software resources!
- You walk out happy to the coffee break...

This talk was mainly based on (self-promote):

- N. (2014): review of fast construction,
- Kuo & N. (2016): QMC4PDE review,
- Magic Point website (and fast CBC construction scripts),
- QMC4PDE website.

But of course there is also L'Écuyer & Munger (TOMS, 2016), Gantner & Schwab's website, Kuo's website.